

Simultaneous retrieval of atmospheric and marine parameters from GEO-CAPE

K. Stamnes^a, W. Li^a, Y. Fan^a, Z. Lin^a, C. Gatebe^b,
B. Hamre^c, K. Sørensen^d, J. J. Stamnes^c

^aLight and Life Laboratory
Department of Physics and Engineering Physics
Stevens Institute of Technology
Hoboken, New Jersey, USA

^bNASA Goddard Space Flight Center, Greenbelt, Maryland, USA

^bUniversities Space Research Association, Columbia, Maryland, USA

^cDepartment of Physics and Technology
University of Bergen, Bergen, Norway

^dNorwegian Institute for Water Research (NIVA)
Oslo, Norway



Outline

- **Background/Motivation**
- **Brief Review of Current Ocean Color Algorithms**
- **Unified Forward/Inverse Modeling Approach:**
 - **Ocean Color – Simultaneous Marine and Aerosol Retrieval Tool (OC-SMART) in Complex, Turbid Environments**
- **Algorithm Overview:**
 - **Nonlinear Optimal Estimation/Levenberg-Marquardt Regularization with a Coupled Atmosphere-Ocean Forward Model**
- **Fast Yet Accurate Retrievals**
 - **Neural Network Training of Forward Radiative Transfer Model**
- **Results**
 - **Synthetic Model Data Validation**
 - **SeaWiFS, MERIS and MODIS Retrievals**
- **GEO-CAPE specific issues**



Background/Motivation

What Can We Do with Ocean Color Data?

Ocean color data can be used for remote evaluation of:

1. water quality;
2. transport of sediments and adhered pollutants;
3. primary production, upon which commercial fish populations depend for food;
4. harmful algal blooms that pose a threat to public health and economies of affected areas.

But reliable retrievals require:

- *accurate characterization of the atmosphere and reliable bio-optical models – challenging problems – especially in turbid coastal waters.*



Light and Life Laboratory
STEVENSONS
Institute of Technology



The Generic Problem: The small ocean signal!

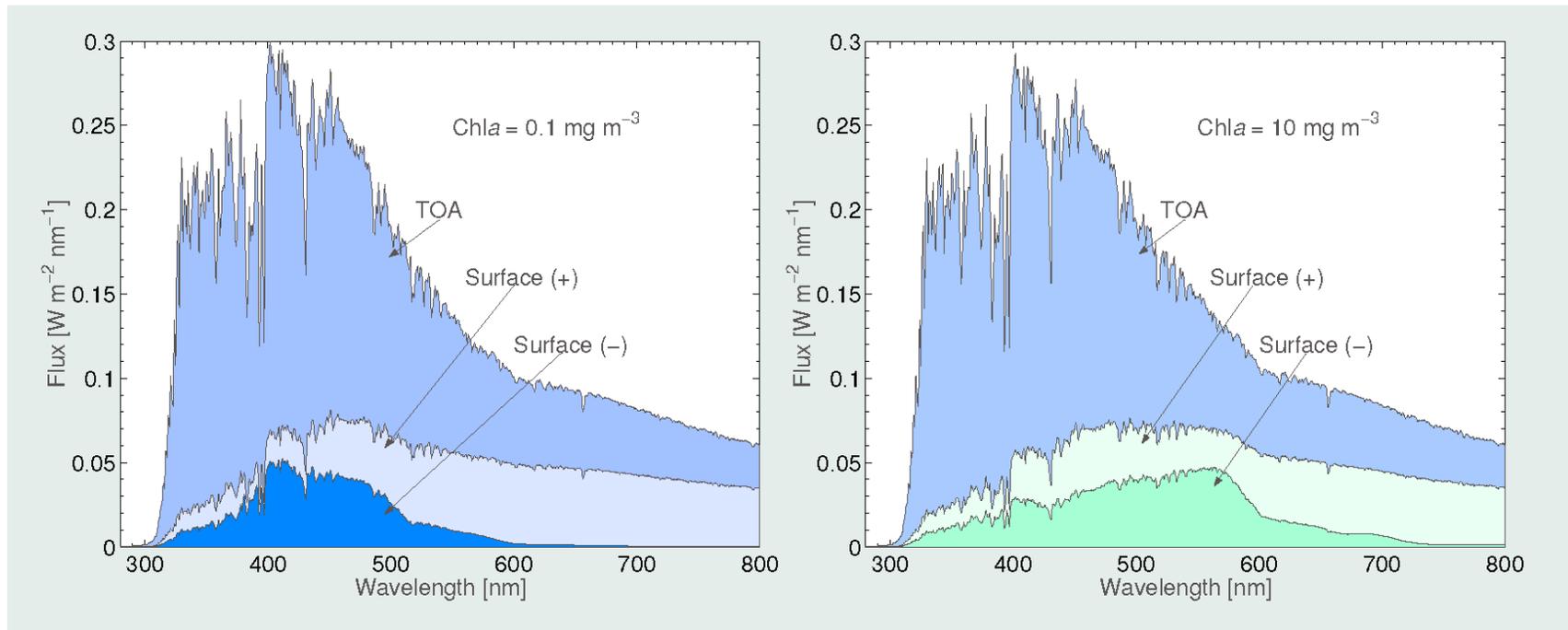


Figure 1: **Left:** Simulated upward irradiance at TOA (upper curve filled with blue color), just above the ocean surface (middle curve filled with light blue color), and just below the ocean surface (lower curve filled with dark blue color). **Right:** Same as left panel, except that the chlorophyll concentration is $\times 100$ larger.

The simulation in the figure above shows that

- there is a **significant change** in sub-surface color with increasing chlorophyll concentration, while at the same time
- there is **only a slight change** in color at the TOA: **the TOA spectra are dominated by light from atmospheric scattering.**

Brief Review of Current Ocean Color Algorithms

Most ocean color algorithms consist of two steps:

1. Do “atmospheric correction” to obtain the water-leaving radiance.
2. Retrieve desired aquatic parameters from the water-leaving radiance.

In the visible more than 90% of the radiance measured by a satellite sensor typically comes from the atmosphere:

- Atmospheric correction becomes a very challenging task **unless the near-infrared (NIR) black-pixel approximation (BPA)** is valid.
- Estimation of diffuse transmittance is also important, but difficult because it depends on the angular distribution of the radiance just beneath the sea surface.

Accurate characterization of the atmosphere – important because:

- a small uncertainty in the atmospheric correction may lead to a big error in the inferred aquatic parameters, and
- aerosol optical properties vary considerably in space and time.



The OC-SMART Approach:

Ocean Color – Simultaneous Marine and Aerosol Retrieval Tool (OC-SMART) in Complex, Turbid Environments Based on Accurate Forward/Inverse Modeling

- Goal: Improve retrieval accuracy by use of AccuRT and Optimal Estimation/Levenberg-Marquardt (OE/LM) inversion:
 - AccuRT: accurate discrete-ordinates radiative transfer model for the *coupled* atmosphere-ocean system; delivers a complete set of simulated radiances and analytically derived Jacobians (weighting functions).
 - OE/LM inversion: nonlinear least squares cost function minimization with *a priori* and Levenberg-Marquardt regularization.
- For retrievals of aerosol and aquatic parameters from Ocean Color data, we define a 5-element state vector:

$$\mathbf{X} = \{\tau_{865}, f, \text{CHL}, \text{CDM}, \text{BBP}\} \longleftarrow \text{state vector.}$$

- 2 aerosol parameters (optical depth at 865 nm, τ_{865} , and bimodal fraction of particles, f),
- 3 marine parameters (chlorophyll concentration, **CHL**, combined absorption by detrital and dissolved material at 443 nm, **CDM**, and backscattering coefficient at 443 nm, **BBP**).



The OC-SMART Approach: Algorithm Overview

At each iteration, next estimate of state vector is given by OE/LM inversion:

$$\mathbf{X}_{n+1} = \mathbf{X}_n + [(1 + \gamma_n)\mathbf{S}_a^{-1} + \mathbf{K}_n^T \mathbf{S}_m^{-1} \mathbf{K}_n]^{-1} \{ \mathbf{K}_n^T \mathbf{S}_m^{-1} (\mathbf{Y}_m - \mathbf{Y}_n) - \mathbf{S}_a^{-1} (\mathbf{X}_n - \mathbf{X}_a) \}.$$

\mathbf{Y}_m = vector of measured TOA radiances,

$\mathbf{Y}_n = F(\mathbf{X}_n, \mathbf{b})$ – vector of simulated TOA radiances generated by the AccuRT forward model; \mathbf{Y}_n is a (non-linear) function of

\mathbf{X}_n – state vector of retrieval elements, \mathbf{b} – model parameters,

\mathbf{K}_n – matrix of simulated radiance partial derivatives w.r.t. state vector elements \mathbf{X}_n (the Jacobians),

\mathbf{X}_a and \mathbf{S}_a are the *a priori* state vector and covariance matrix, respectively,

\mathbf{S}_m is the measurement error covariance.

- γ_n is the Levenberg-Marquardt (LM) regularization parameter:
 $\gamma_n = 0 \Rightarrow$ Gauss-Newton Optimal Estimation (OE).
- AccuRT returns simulated radiances (\mathbf{Y}_n) and Jacobians (\mathbf{K}_n) required to update the state vector estimate (\mathbf{X}_n) according to the equation above.



The OC-SMART Approach:

Inherent Optical Properties (IOPs) – Bio-optical Model

The IOPs are based on simple wavelength-dependent parameterizations of:

$$a_{ph}(\lambda) = \alpha_1(\lambda) \mathbf{CHL} \alpha_2(\lambda) \quad \longleftarrow \quad \text{phytoplankton abs. coeff.} \quad (1)$$

$$a_{dg}(\lambda) = \mathbf{CDM} e^{[-S(\lambda-\lambda_0)]} \quad \longleftarrow \quad \text{detrital and diss. material abs. coeff.} \quad (2)$$

$$b_{bp}(\lambda) = \mathbf{BBP} (\lambda/\lambda_0)^{-\eta} \quad \longleftarrow \quad \text{backscatter coeff.} \quad (3)$$

in terms of the values of $\mathbf{CDM} \equiv a_{dg}(\lambda_0)$ and $\mathbf{BBP} \equiv b_{bp}(\lambda_0)$ at some reference wavelength λ_0 . Thus, the bio-optical model is described by:

- the three retrieval elements $\{\mathbf{CHL}, \mathbf{CDM}, \mathbf{BBP}\}$, and
- the four model parameters $\{\alpha_1(\lambda), \alpha_2(\lambda), S, \eta\}$;
- $\alpha_1(\lambda)$ and $\alpha_2(\lambda)$ are determined by fitting Eq. (1) to field measurements of chlorophyll absorption (using *e.g.* NOMAD data base).
- Values for S , η and pure water absorption and scattering coefficients $a_w(\lambda)$ and $b_w(\lambda)$ are adopted from the literature.
- For pure water scattering we use the **Rayleigh phase function**, and for particulate scattering the analytic **Fournier-Forand phase function**.



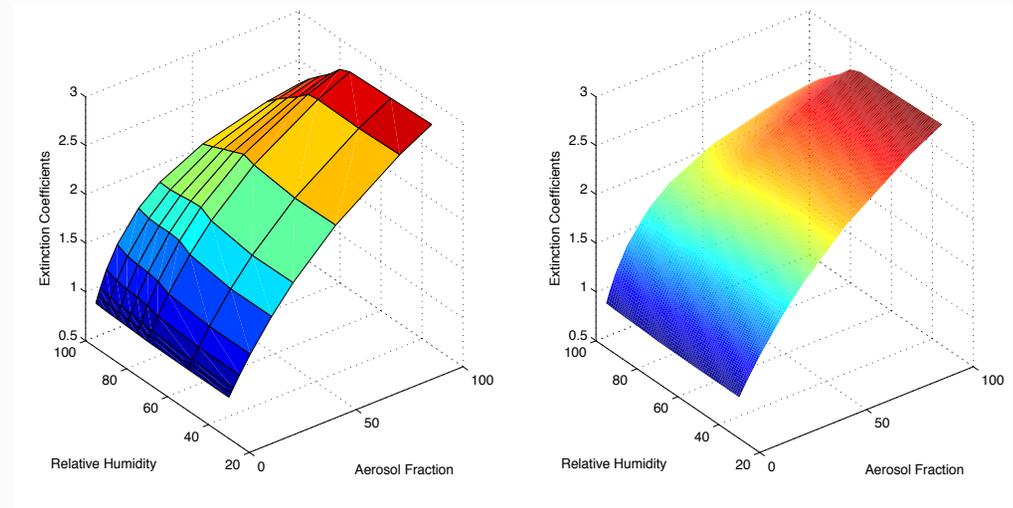
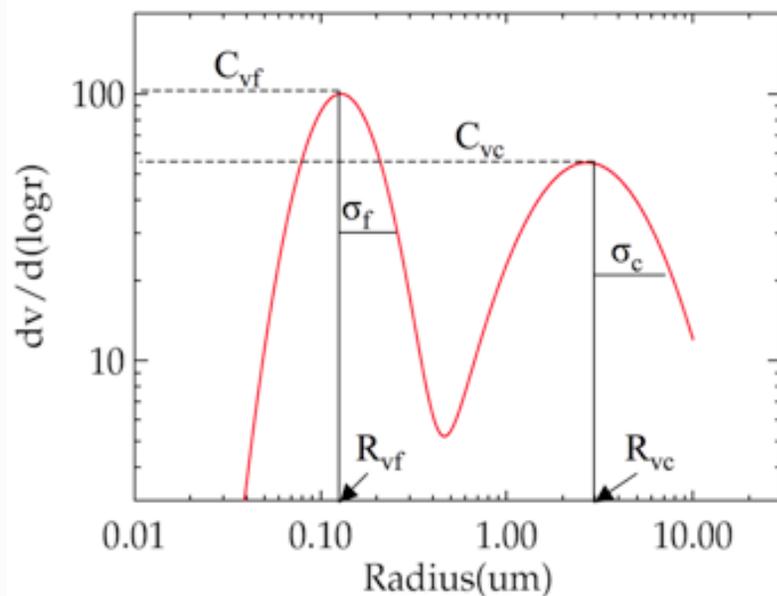
The OC-SMART Approach: Aerosol IOPs: SeaDAS Aerosol Models

We use the 80 SeaDAS aerosol models based on AERONET data (Ahmad et al., 2010).

2 aerosol retrieval parameters:

τ : aerosol optical depth at 865nm.

F: aerosol fraction.



MODIS aerosol extinction coefficients at 555 nm

10 different aerosol fractions: 0, 1, 2, 5, 10, 20, 30, 50, 80, 95

8 different relative humidities: 30, 50, 70, 75, 80, 85, 90, 95

The OC-SMART Approach: SeaWiFS Image Retrieval at SBC

- As an example we consider a SeaWiFS image of the Santa Barbara Channel, obtained on Feb. 28, 2003, and
- Use the OC-SMART forward and inverse model for simultaneous retrieval of the 5-element state vector:

$$\mathbf{X} = \{\tau_{865}, f, \text{CHL}, \text{CDM}, \text{BBP}\} \leftarrow \text{state vector.}$$

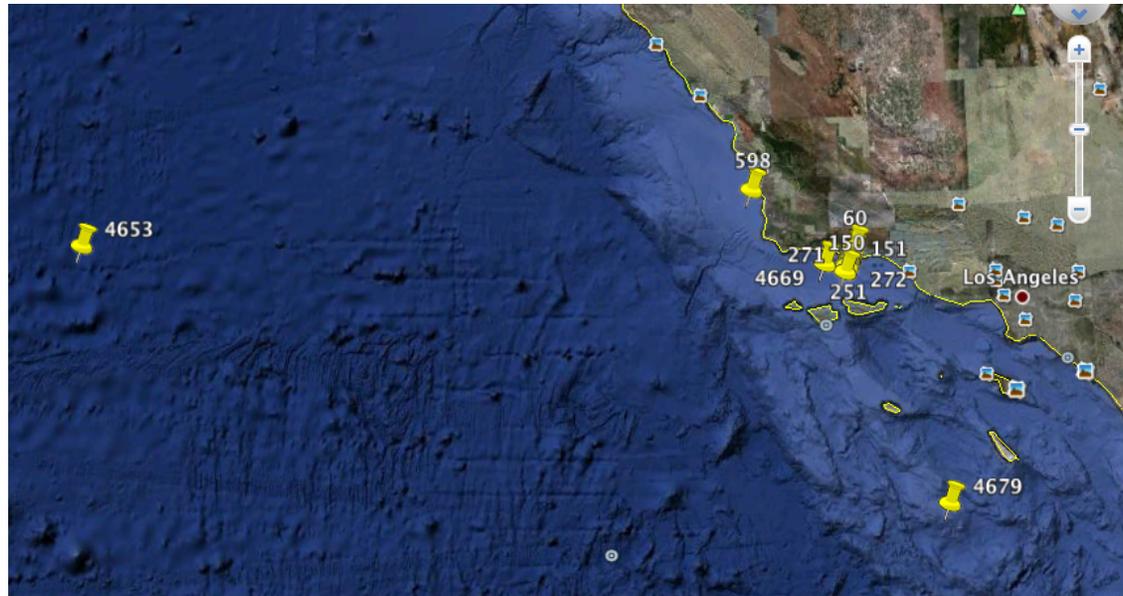
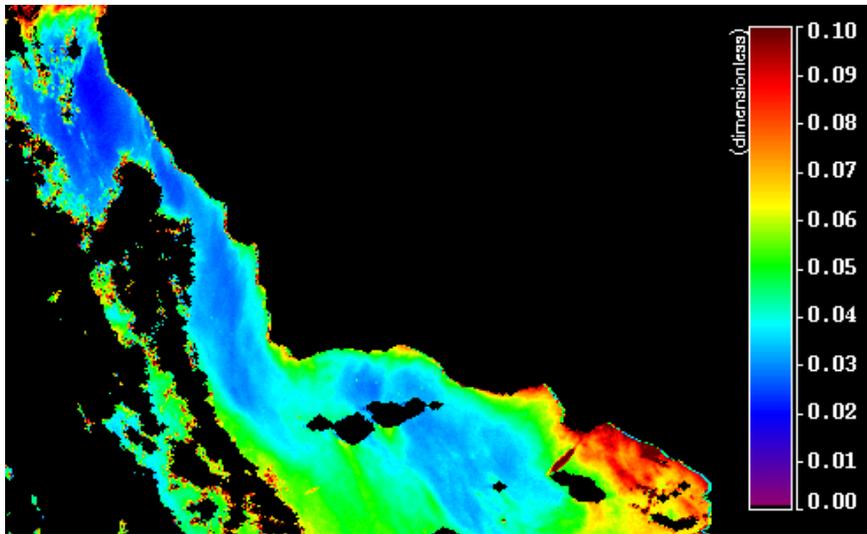
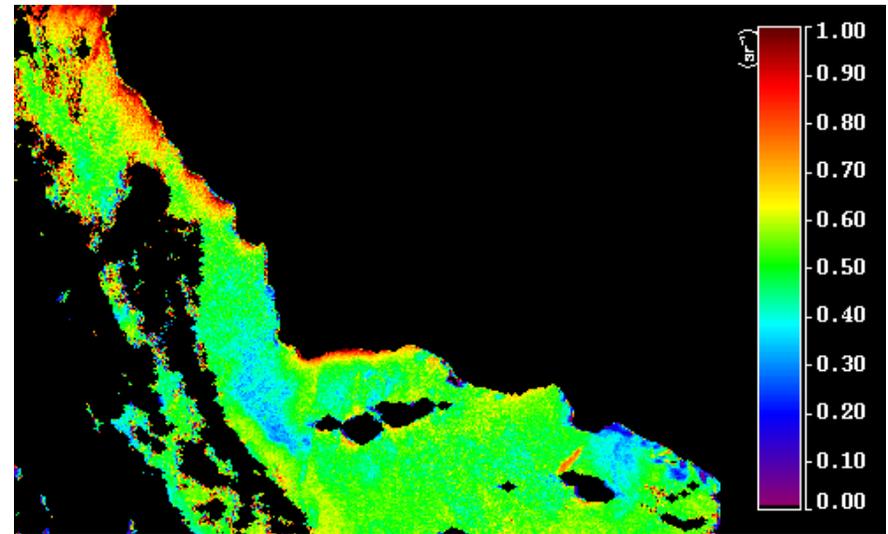


Figure 2: Map showing locations of Southern California sites.

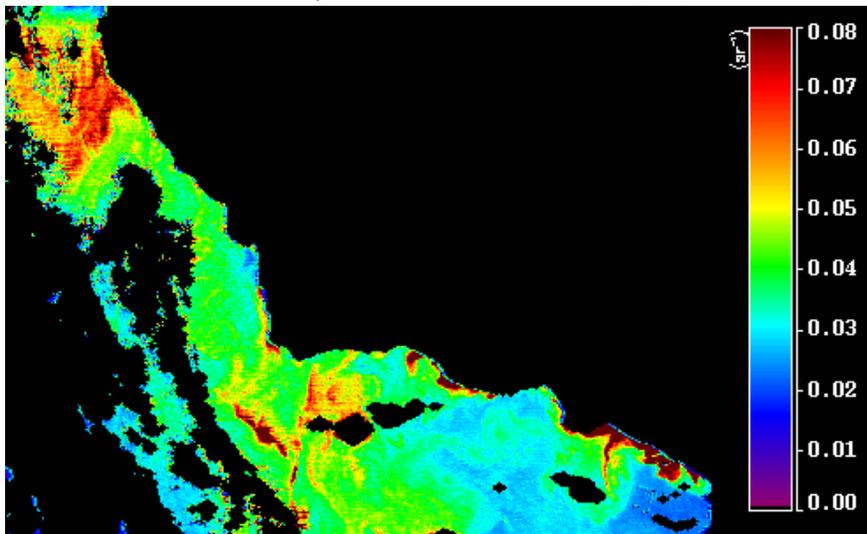
Aerosol optical depth at 865nm



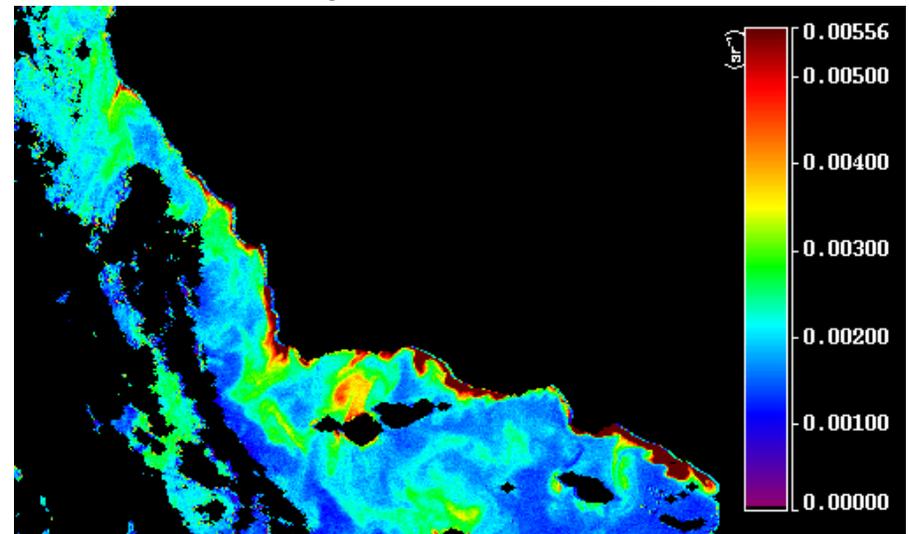
Bimodal fraction of aerosol particles

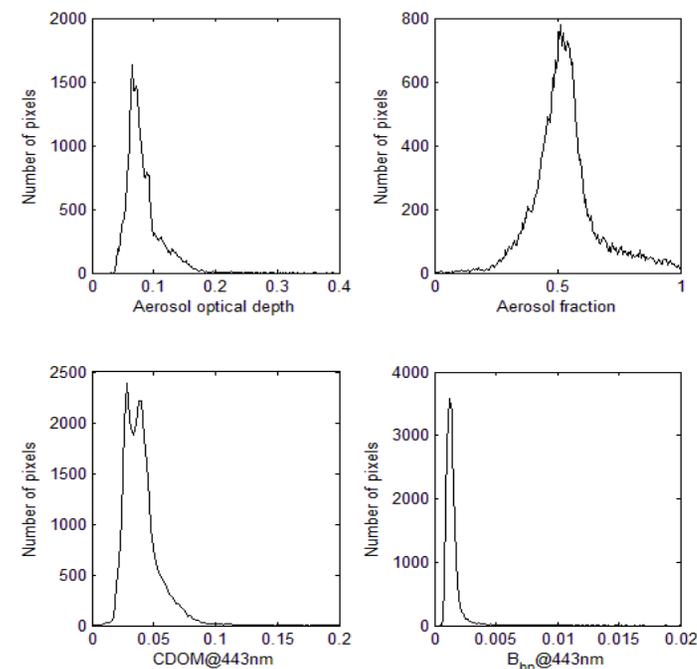
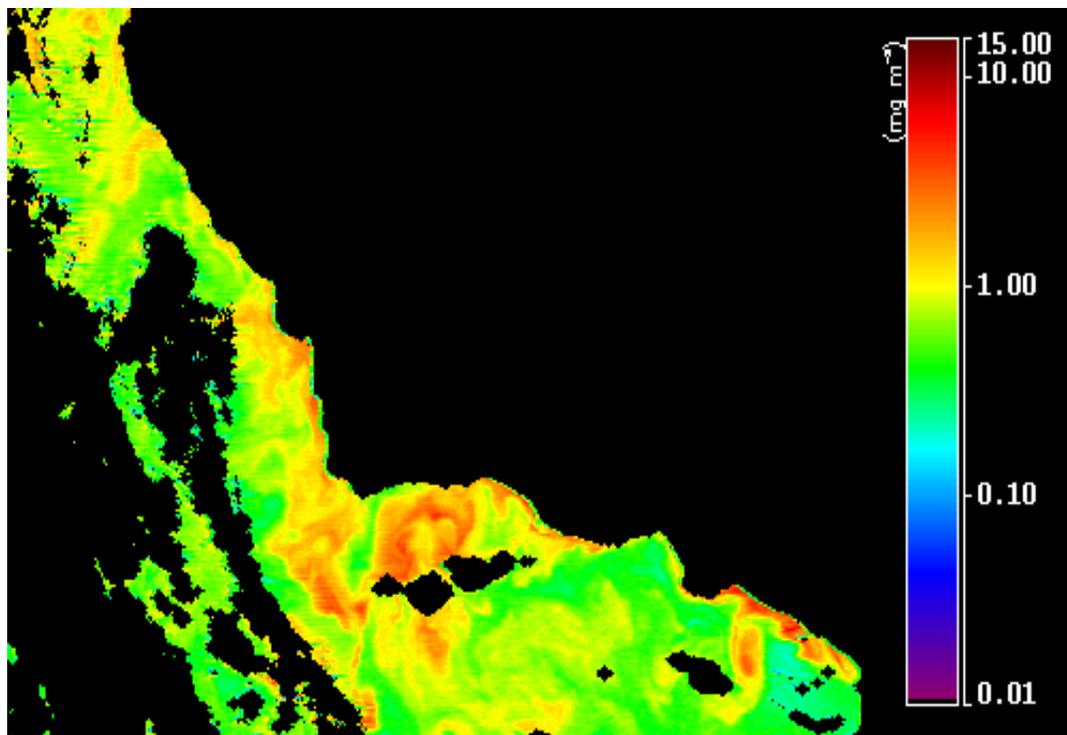


CDOM absorption coefficient at 443nm (m⁻¹)



Backscattering coefficient at 443nm (m⁻¹)





Left panel: Retrieved chlorophyll concentration ($\text{mg} \cdot \text{m}^{-3}$) from SeaWiFS image on Feb. 28, 2003 over the Santa Barbara Channel.

Right top panel: The distributions of the other retrieved parameters from the same image. (a) aerosol optical depth; (b) aerosol model fraction; (c) CDOM absorption coefficient at 443nm (m^{-1}); (d) backscattering at 443nm (m^{-1})

Right bottom table: Radiance residuals at all SeaWiFS channels.

Wavelength	Average relative error (%)	Pixels with <2% relative error (%)
412nm	± 0.298	99.488
443nm	± 0.289	99.625
490nm	± 0.555	99.216
510nm	± 0.716	98.552
555nm	± 0.240	99.168
670nm	± 1.050	94.267
765nm	± 1.952	64.102
865nm	± 0.857	94.745

The OC-SMART Approach: Lessons Learned

Examination of about 35,000 pixels in the SBC SeaWiFS image showed that:

- the residuals were less than 1% for 7 of the 8 SeaWiFS channels, and less than 2% for the remaining 765 nm (O₂ A-band) channel.

We conclude that:

- OC-SMART appears to yield very good retrieval capability: 8 SeaWiFS channels are sufficient to retrieve 2 atmospheric and 3 marine parameters in coastal waters.

In addition to well-calibrated SeaWiFS data, the good retrievals are believed to be due to:

- The availability of high quality field data, which were used to construct a reliable bio-optical model.
- An aerosol model with an *adjustable* bimodal fraction of large versus small particles.



The OC-SMART Approach: *Speeding up the Forward Model*

- We have just demonstrated that the OC-SMART retrieval algorithm can be used to retrieve the 5-element state vector:

$$\mathbf{X} = \{\tau_{865}, f, \text{CHL}, \text{CDM}, \text{BBP}\} \longleftarrow \text{state vector.}$$

but the algorithm is fairly slow!!

- The most time-consuming step in the inversion process is the AccuRT forward model computations.
- However, it is possible to reach operational speed with a fast forward model that is obtained by using AccuRT to train a Radial-Basis-Functions Neural Network (RBF-NN).
- Speed enhancement $\sim 1,500$.
- On an ordinary table top computer, it takes < 2 minutes to analyze $\sim 35,000$ pixels using the fast RBF-NN forward model.



The OC-SMART Approach: *Fast Forward Model*

Use AccuRT to create a training ensemble to construct **RBF-NN**'s to

- replace the AccuRT forward model (thousands of lines of code) with the following single equation:

$$L_i = \sum_{j=1}^N a_{ij} \exp\left[-b \sum_{k=1}^K (P_k - c_{jk})^2\right] + d_i \quad \leftarrow \quad \mathbf{RBF - NN's}$$

L_i = TOA radiance in channel $i = 1, \dots, 8$, $K = \#$ of input parameters
 $a_{i,j}, b, c_{j,k}, d_i$ = coefficients to be optimized.

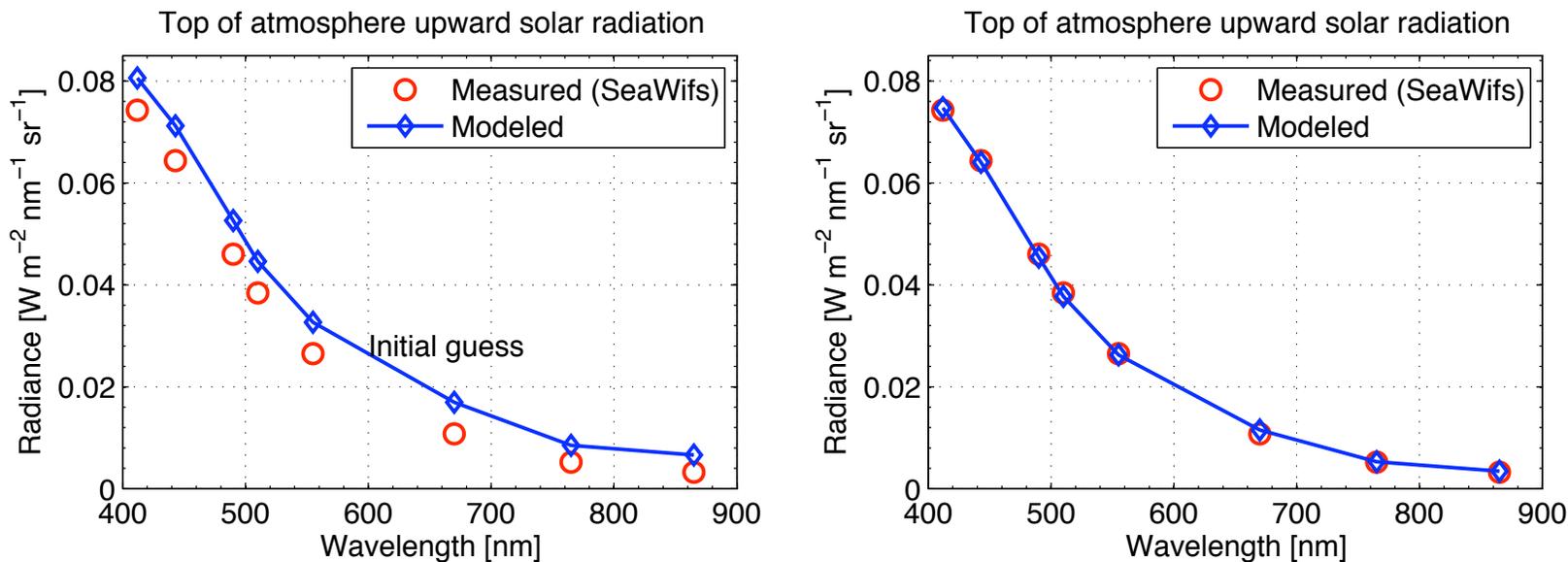


Figure 3: **Left: Initial guess. Right: Third iteration: Converged Result.**

OC-SMART: Salient Features

- AccuRT provides accurate radiances at TOA and BOA.
- OC-SMART can estimate residuals and thus check the quality of the retrievals through “self-evaluation” of retrieved parameters (error budgets) – 2-step validation must rely exclusively on sparsely available field data.
- OE/LM inverse method provides simultaneous retrieval of aerosol and marine parameters:
 $\mathbf{X} = \{\tau_{865}, f, \text{CHL}, \text{CDM}, \text{BBP}\} \leftarrow \text{state vector.}$
- Aerosol model and bio-optical model can be easily changed, which is valuable because:
 - a given coastal region may require a *local* marine bio-optical model to represent water IOPs, and a *local* aerosol IOP model.
- RBF-NN training of RTM provides fast yet accurate retrievals.
- OC-SMART has already been applied to different sensors, including MERIS, MODIS, and SeaWiFS and to low solar elevation data.



GEO-Cape issues:

1. Low solar elevations

The **plane parallel approximation (PPA)** breaks down for solar zenith angles larger than about 70°. How do we proceed?

- One option: use the **pseudo-spherical approximation (PSA)** [Eq. (4)]:
 - the direct beam single scattering (solar pseudo-source) term is treated in spherical geometry: $e^{-\tau/\mu_0} \rightarrow e^{-\tau Ch(r,\mu_0)} \leftarrow$ **PSA**
 - while the multiple scattering term is treated using the PPA:

$$\begin{aligned}
 \mu \frac{dL(\tau, \mu, \phi)}{d\tau} = & L(\tau, \mu, \phi) - \underbrace{\frac{\varpi(\tau)}{4\pi} \int_0^{2\pi} d\phi' \int_{-1}^1 d\mu' p(\tau, \mu', \phi'; \mu, \phi) L(\tau, \mu', \phi')}_{\text{multiple scattering}} \\
 & \underbrace{- \frac{\varpi(\tau)}{4\pi} p(\tau, -\mu_0, \phi_0; \mu, \phi) F^s e^{-\tau Ch(\mu_0)}}_{\text{single scattering}}. \tag{4}
 \end{aligned}$$



Advantage of using the pseudo-spherical approximation

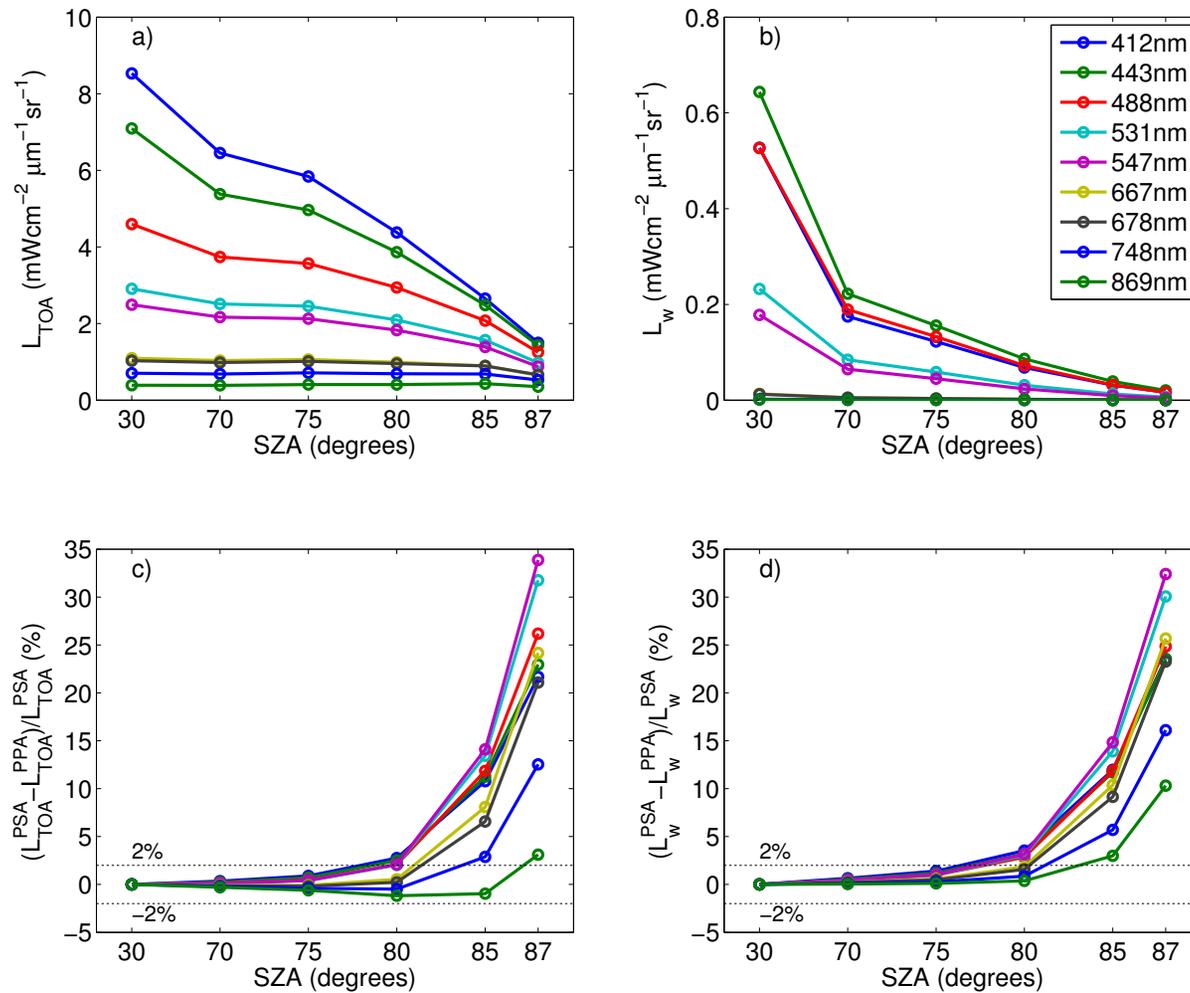


Figure 4: a) TOA radiance (L_{TOA}) and c) relative difference incurred by using plane-parallel geometry (PPA) for several values of solar zenith angle (SZA) between 30° and 87° . b) Same as for a) but for the water-leaving radiance and d) relative difference incurred by using PPA. Viewing geometry: $\phi = 120^\circ$; $\tau_a(865) = 0.05$. Fraction of small vs. large aerosol particles was set to 0.5. Water bio-optical properties: Chla = 0.1 mg m^{-3} , colored detrital absorption coefficient at 443 nm = 0.05 m^{-1} , particulate backscattering coefficient at 443 nm = 0.001 m^{-1} .

2. Advantage of using a 2-D Gaussian distribution of surface slopes

What about the lower boundary: 1-D or 2-D Gaussian?

Explore advantage of using a 2-D Gaussian distribution of surface slopes?

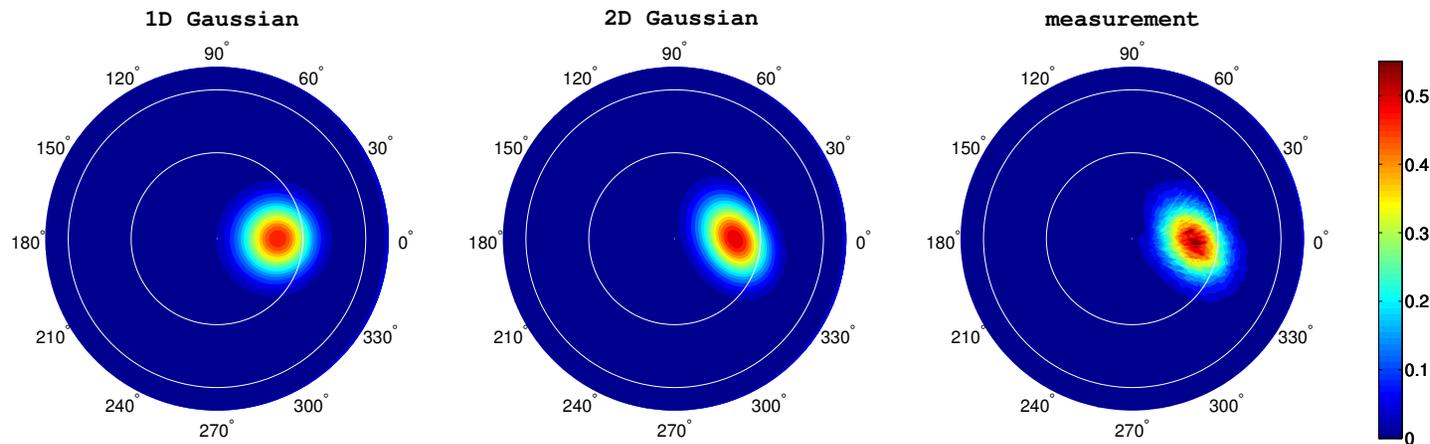


Figure 5: Comparison of reflectances for model simulations assuming a 1-D Gaussian BRDF (left), a 2-D Gaussian BRDF (middle), and measurements (right).

Use of

- (1) a 2-D Gaussian surface slope distribution for singly scattered light, and
 - (2) a 1-D Gaussian surface slope distribution for multiply scattered light
- is quite successful because the 2-D BRDF simulates the sunglint very well, while the 1-D BRDF is sufficient to simulate the smoother sky reflectance.

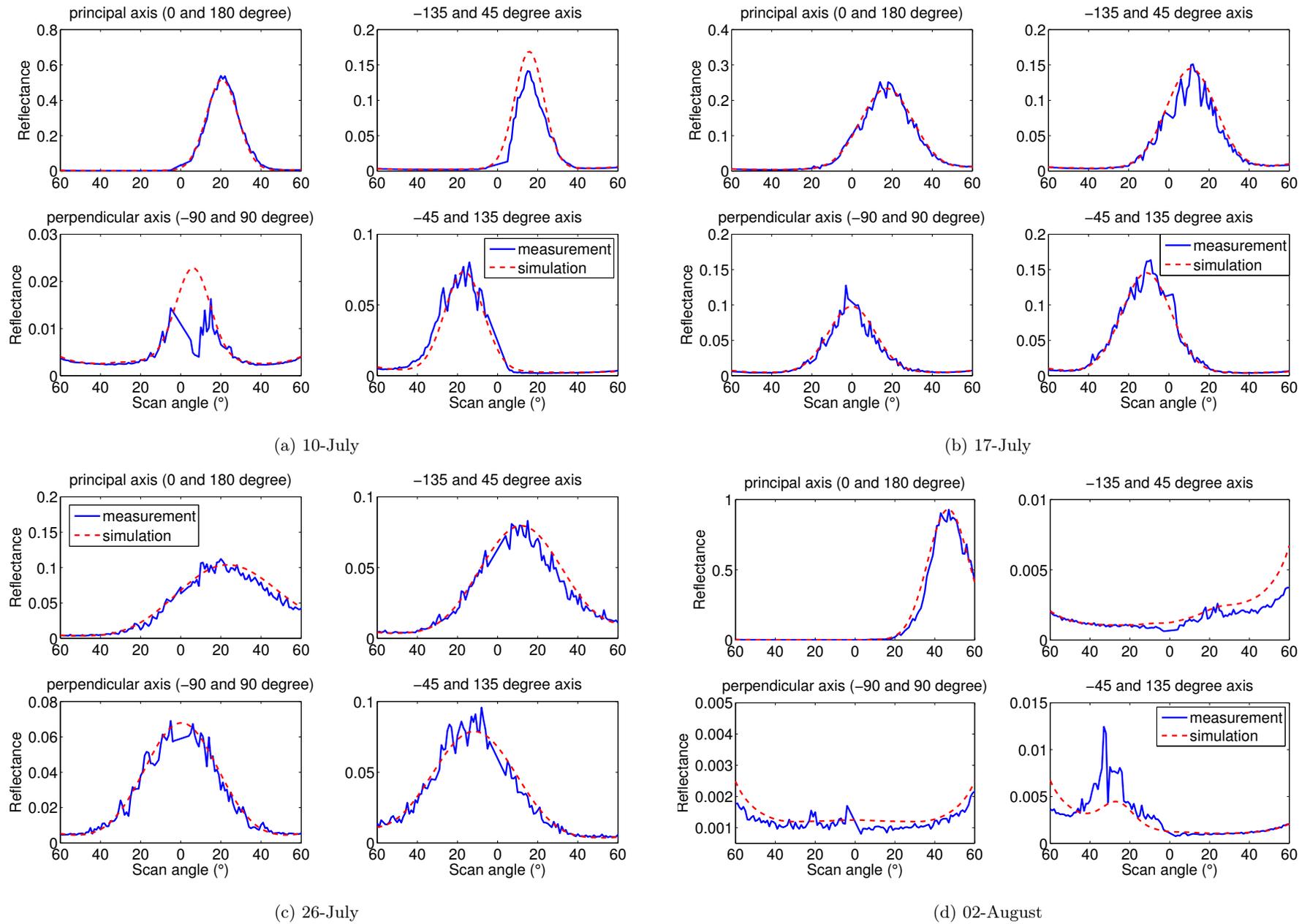
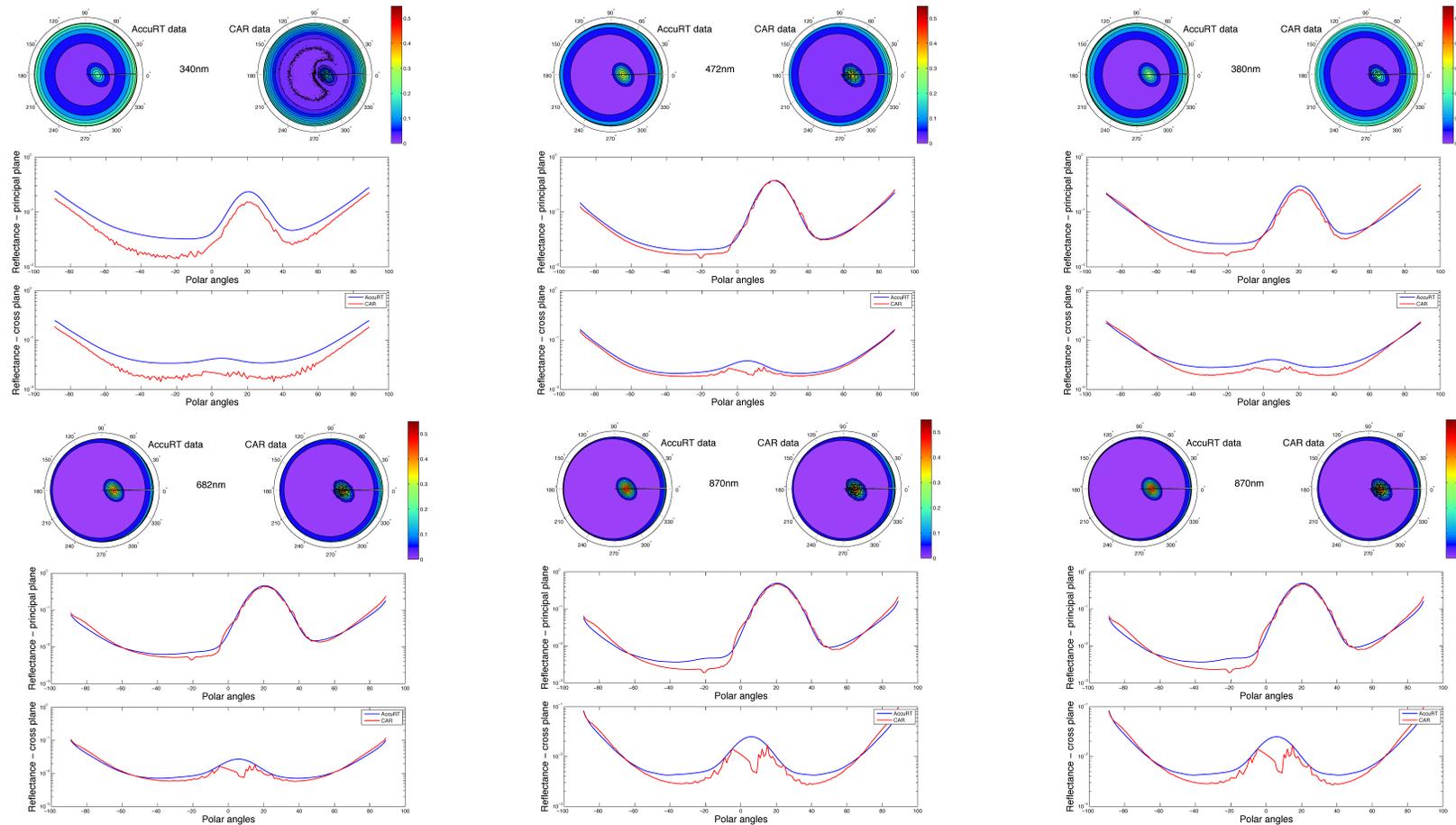


Figure 6: Comparison between model-simulated and measured reflectances for different geometries.

Validation of the BRDF and 2D Sun Glint Model with CAR Data

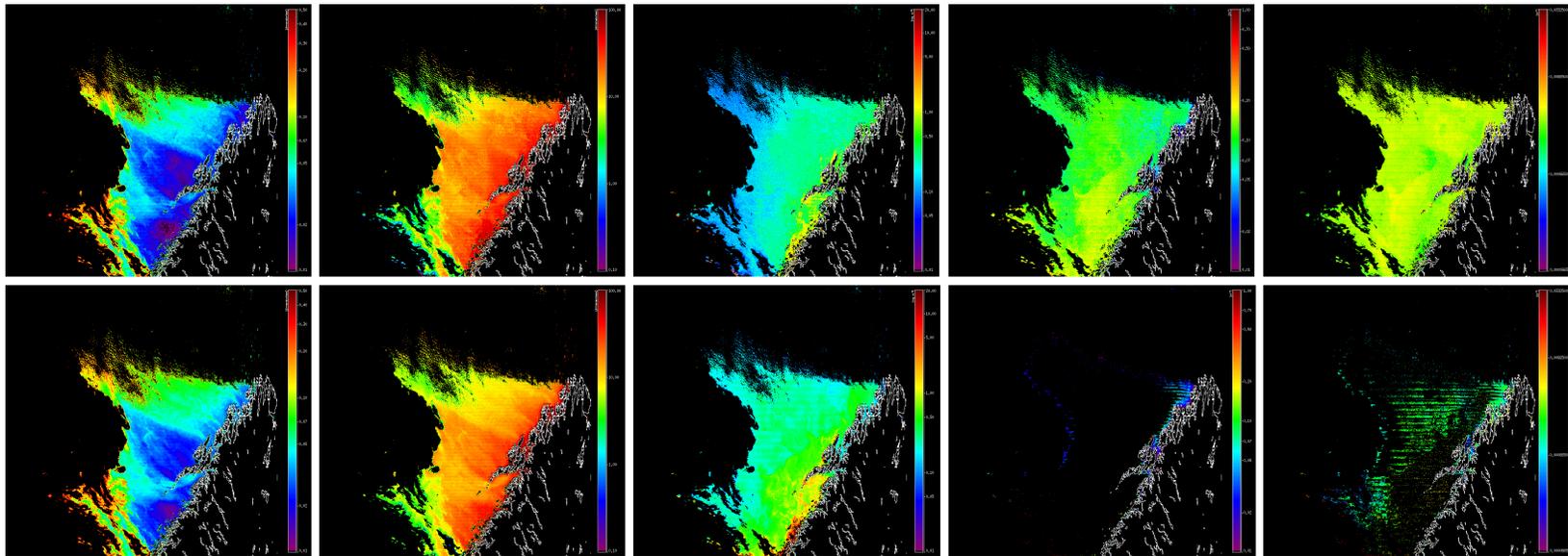


Comparison between simulated (blue) and CAR measured surface reflectance (red). Upper panels: 340, 380, and 472 nm. Lower panels: 682, 870 and 1036 nm. Within each panel, the top display shows a comparison of the entire surface reflectance, the middle curves show the comparison of a line of data extracted from the principal plane, and the bottom curves show the same as the middle curves but from 90° across the principal plane.

3. Standard ocean color algorithms do not work well in coastal areas

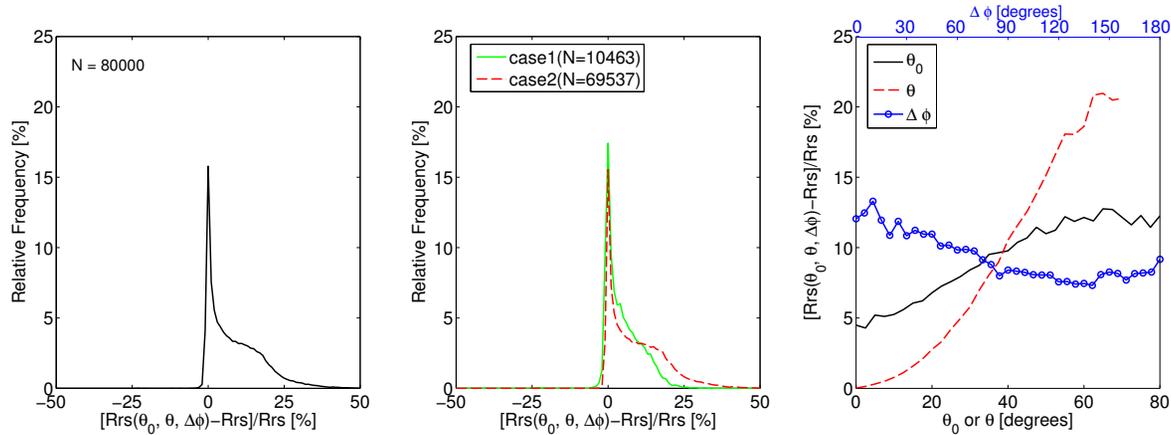
Below (lower panels) is an example of the problem caused by the infamous **negative** water-leaving radiance problem due to failure of the atmospheric correction.

- Can the failing atmospheric correction be fixed? Or should it be
- entirely avoided by using **simultaneous atmosphere/ocean retrieval** based on RT models for the coupled atmosphere/ocean system (upper panels)?

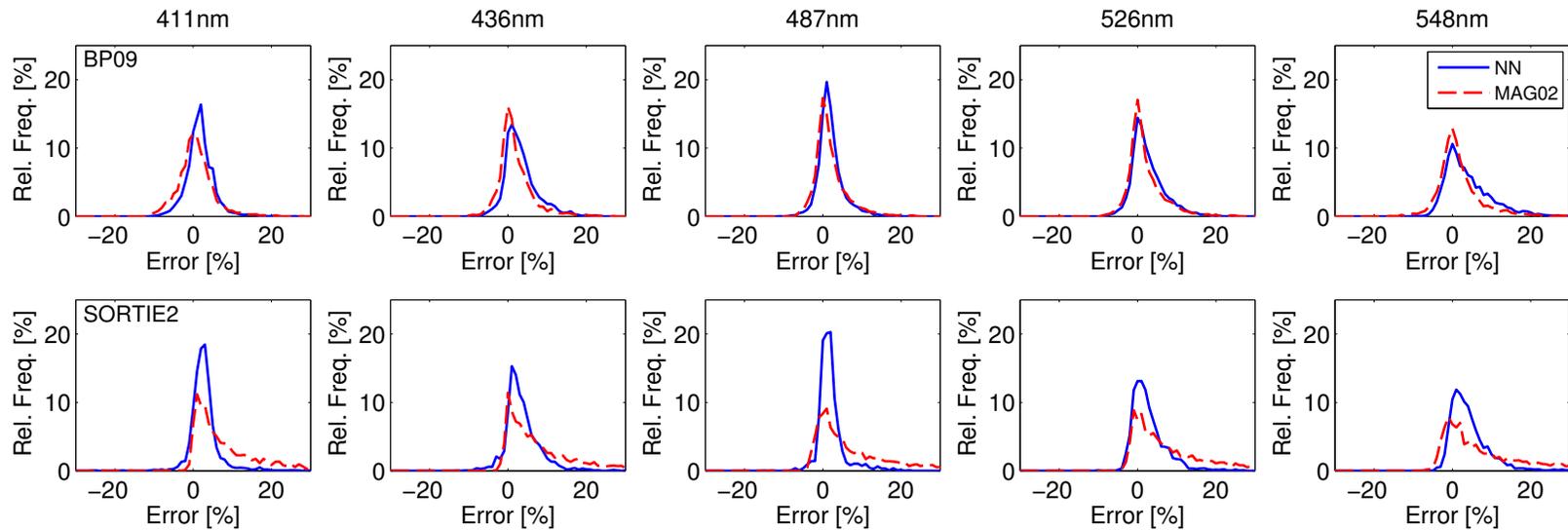


Comparison between **simultaneous** (OC-SMART, top) and **standard** (SeaDAS, bottom) retrievals for a MODIS image on 04/18/2014 over a coastal area in northern part of Norway. From left to right: τ_{869} , f , CHL, CDOM and b_{bp} , respectively.

4. Improved BRDF corrections in coastal waters using NN method



Panel 1: percentage difference between viewing angle-dependent $R_{rs}(\theta_0, \theta, \Delta\phi)$ and nadir viewing $R_{rs}(\theta_0)$ values. Panel 2: distribution of the difference for Case 1 and Case 2 waters. Panel 3: dependence on sun-sensor geometry.



Comparison of the percentage error distribution of the BRDF derived from the NN and MAG02 algorithms. Upper panel: Chlorophyll-dominated waters (Ligurian Sea). Lower panel: Case 2 waters (San Diego Bay).

Final thought: What about using vector (polarized) RT simulations?

- Preliminary results indicate that even for **radiance-only** measurements:
- the accuracy of the retrievals could be improved by using a vector (polarized) forward RT model to compute the radiances used in the inversion step.

Hence, for GEO-CAPE ocean color retrievals:

- It might be worthwhile exploring the advantage of using the pseudo-spherical approximation combined with polarized (vector) radiative transfer simulations and a 2-D Gaussian distribution of surface slopes.



Further reading?

WILEY-VCH

WILEY-VCH

This book discusses radiative transfer in coupled media such as atmosphere-ocean systems with Lambertian as well as non-Lambertian reflecting surfaces at the lower boundary.

The spectral range from the ultraviolet to the microwave region of the electromagnetic spectrum is considered, and multi-spectral as well as hyperspectral remote sensing is discussed. Solutions of the forward problem for unpolarized and polarized radiation are discussed in considerable detail, but what makes this book unique is that formulations and solutions of the inverse problem related to such coupled media are covered in a comprehensive and systematic manner.

This book teaches the reader how to formulate and solve forward and inverse problems related to coupled media, and gives examples of how to solve concrete problems in environmental remote sensing of coupled atmosphere-surface systems.

From the contents:

- Inherent Optical Properties (IOPs)
- Basic Radiative Transfer Theory
- Forward Radiative Transfer Modeling
- The Inverse Problem
- Applications



Knut Stamnes is professor of physics in the Department of Physics and Engineering Physics, and Director of the Light and Life Laboratory at Stevens Institute of Technology in Hoboken New Jersey. Stamnes began his career in upper atmospheric physics, and has since specialized in atmospheric radiation, remote sensing, and climate-related studies. He is a fellow of the OSA, a member of the AGU, EGU, and SPIE, and was elected member of the Norwegian Academy of Technological Sciences in 2009.



Jakob J. Stamnes is professor of physics in the Department of Physics and Technology at the University of Bergen, Norway. He is fellow of the OSA, founding member and fellow of the EOS (European Optical Society), a member of the SPIE, EGU, and the Norwegian Physical Society, and was elected member of the Norwegian Academy of Technological Sciences in 2009.

www.wiley-vch.de

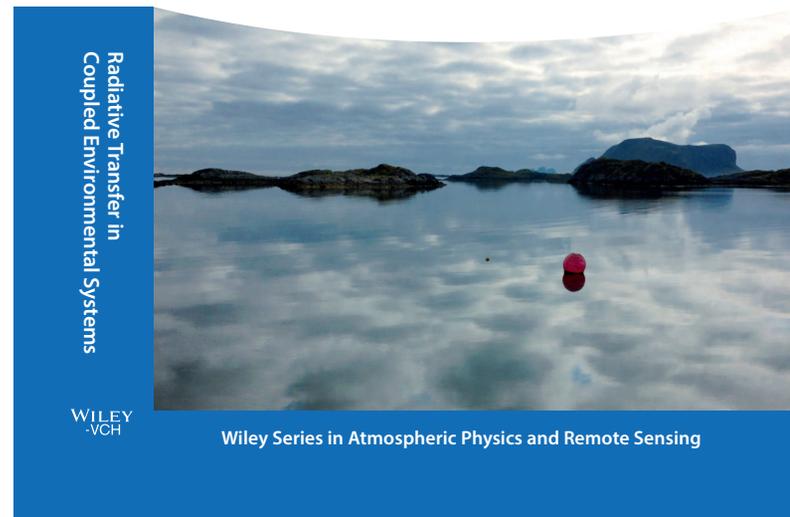


Stamnes • Stamnes

Knud and Jakob Stamnes

Radiative Transfer in Coupled Environmental Systems

An Introduction to Forward and Inverse Modeling



WILEY-VCH

Wiley Series in Atmospheric Physics and Remote Sensing

THANK YOU FOR YOUR ATTENTION!



Light and Life Laboratory

STEVENS
Institute of Technology

